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INTRINSIC CHIRALITY OF COMPLETE GRAPHS

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ABSTRACT. A graph is said to be intrinsically chiral if no embedding of the graph in 3-space is respected by any ambient orientation-reversing homeomorphism. In this note, we characterize those complete graphs that are intrinsically chiral.

It is often important in predicting chemical properties to know whether a molecule is distinct from its mirror image. A molecule that cannot convert itself into its own mirror image is said to be *chemically chiral*. Mathematically, we consider the molecule as a graph in 3-space and ask whether there is an orientation-reversing homeomorphism that takes the graph to itself. A graph embedded in 3-space is said to be *achiral* if there exists such a homeomorphism and *chiral* if there is no such homeomorphism. Note that a molecule whose corresponding graph is chiral is necessarily chemically chiral.

Given that some particular embedding of a graph in 3-space is chiral, it is natural to ask whether it is possible to reembed the graph in such a way that it is now achiral, or whether the chirality is intrinsic to the graph. If there exists some achiral embedding of a graph G, we say that G is *achirally embeddable*; otherwise, we say that G is *intrinsically chiral*.

The *complete graph on* n *vertices* is defined as a set of n vertices together with an edge between each pair of vertices. In this note, we characterize those complete graphs that are intrinsically chiral. In particular, we prove the following

Theorem. *The complete graphs* K_{4n+3} *with* $n \geq 1$ *are intrinsically achiral. All other complete graphs* K_n *are achirally embeddable.*

First we demonstrate that the complete graphs other than K_{4n+3}, $n \geq 1$, are achirally embeddable. We do this by actually exhibiting achiral embeddings. The complete graphs K_1, K_2, and K_3 are planar, and the construction is therefore trivial for them. The next case consists of all graphs K_{4n}, $n \geq 1$, for which we will give a general form by

Proposition 1. *Let* G *be a finite graph for which there exists an order* 4 *automorphism* $\alpha : G \to G$ *such that the orbit of every vertex under* α *has length* 4. *Then* G *is achirally embeddable.*

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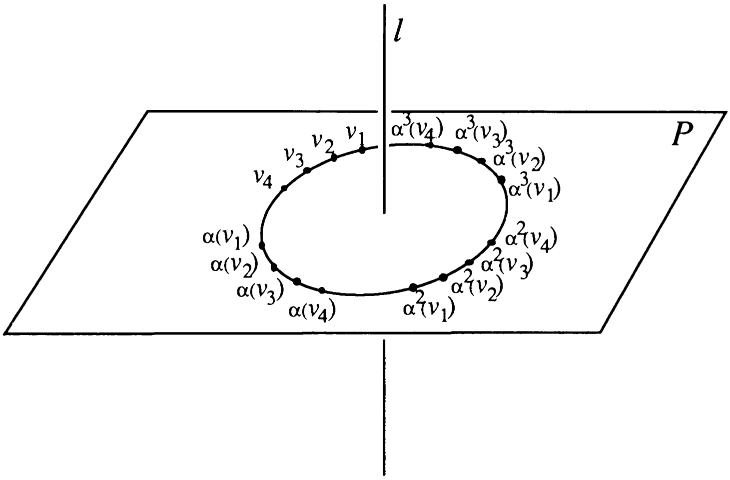

FIGURE 1

Proof. Place the vertices of G on a circle C in a horizontal plane $P \subset \mathbb{R}^3$ so that the $90°$ rotation about a perpendicular line l induces the same permutation of vertices as α (see Figure 1). Let $f : \mathbb{R}^3 \to \mathbb{R}^3$ be the composition of the $90°$ rotation about l with the reflection through the plane P.

Choose $e_1, \dots, e_p$ to be representatives from each edge orbit. Then choose ellipsoids $E_1, \dots, E_p$ that are symmetric about l and P and meet at the circle C containing the vertices, as in Figure 2. We now embed the edges of G as follows.

The edge e_i is invariant under α^2 if e_i joins a vertex v to $\alpha^2(v)$. In this case, embed e_i in the upper half-ellipsoid E_i^+ so that it is invariant under the $180°$ rotation f^2 about l. (For instance, take e_i to be the intersection of E_i^+ with a vertical plane.) And embed $\alpha(e_i)$ as the image of this edge under f, contained in the lower half-ellipsoid E_i^-.

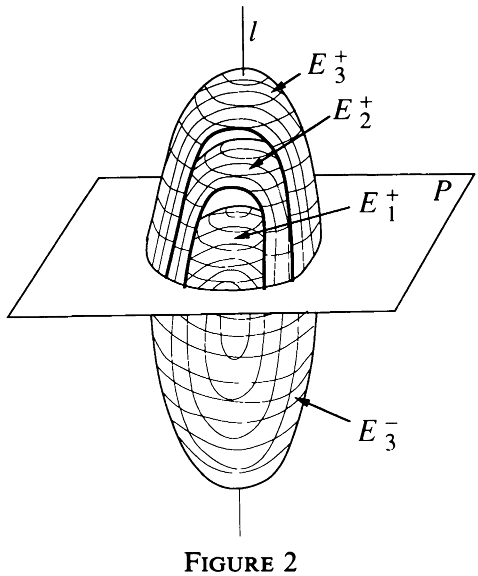

FIGURE 2

Suppose e_i is not invariant under α^2. Then e_i joins a vertex v to a vertex w and v and w are not antipodal points on the circle C. Consider the semi-circles A and B of C with end points v and $\alpha^2(v)$, the antipodal point of v. Without loss of generality, v and w are both contained in A. Hence, $\alpha^2(v)$ and $\alpha^2(w)$ are both contained in B. Thus an edge joining v to w in the half-ellipsoid E_i^+ does not need to meet an edge joining $\alpha^2(v)$ to $\alpha^2(w)$. So, embed e_i in E_i^+ so that it is disjoint from its image under f^2 (again, the intersection of E_i^+ with a vertical plane will do). Embed $\alpha(e_i)$, $\alpha^2(e_i)$, $\alpha^3(e_i)$ as the images of e_i under f, f^2, f^3, respectively.

We now have specified an embedding of G in $\mathbb{R}^3$, which is invariant under the orientation-reversing homeomorphism $f: \mathbb{R}^3 \to \mathbb{R}^3$. This proves that G is achirally embeddable.

Corollary. *For every $n \geq 1$, K_{4n} is achirally embeddable.*

Proposition 2. *For every $n \geq 1$, K_{4n+1} is achirally embeddable.*

Proof. First carry out the construction of the proof of Proposition 1 to embed a subgraph K_{4n} of K_{4n+1} in $\mathbb{R}^3$. Then add the final vertex at the point where the plane P intersects the line l, with straight edges connecting this vertex to all the other vertices. The same homeomorphism f now takes the embedded K_{4n+1} to itself, showing that the embedding is achiral. □

Proposition 3. *For every $n \geq 1$, K_{4n+2} is achirally embeddable.*

Proof. Embed a subgraph K_{4n} of K_{4n+2} as in the proof of Proposition 1. Let E_0 be an additional symmetric ellipsoid that is contained in the interior of all the other E_i. Then add the remaining two vertices at $l \cap E_0^+$ and $l \cap E_0^-$. Connect these last two vertices to each other by a line segment in l and to the other $4n$ vertices by intersections of $E_0^\pm$ with vertical planes. Once again, the homeomorphism f still takes this embedded K_{4n+2} to itself, showing that the embedding is achiral. □

To prove that K_{4n+3} is intrinsically chiral when $n \geq 1$, we start with a

Lemma. *Let $f: \mathbb{R}^3 \to \mathbb{R}^3$ be a homeomorphism that respects an embedding of K_7 in $\mathbb{R}^3$. If the action of f on the vertices of K_7 has order 2 then f fixes exactly one vertex.*

Proof. Our proof is based on a result of Conway and Gordon [CG]. Let a *7-loop* in K_7 be any subgraph that is homeomorphic to a circle and passes through all 7 vertices of K_7. Given an embedding of K_7 in $\mathbb{R}^3$, such a 7-loop c forms a (possibly trivial) knot in $\mathbb{R}^3$, and therefore has a well-defined *Arf invariant* $a(c) \in \mathbb{Z}_2$ (see for instance the appendix of [CG] for the definition of the Arf invariant). Conway and Gordon prove that the $\mathbb{Z}_2$ – sum $\sum_{c \in \mathscr{C}} a(c)$, where c ranges over the set $\mathscr{C}$ of all 7-loops in K_7, is always equal to 1.

Now f acts as an involution on the set $\mathscr{C}$. Since f is a homeomorphism of $\mathbb{R}^3$, $a(f(c)) = a(c)$ for every $c \in \mathscr{C}$. Pairing each $c \in \mathscr{C}$ with its image, we conclude that $1 = \sum_{c \in \mathscr{C}} a(c) = \sum_{f(c)=c} a(c)$. In particular, f respects some $c_0 \in \mathscr{C}$. This means that it is possible to choose a 7-tuple of distinct vertices of K_7 so that f acts on this 7-tuple either by a cyclic permutation or by reversing its order. A cyclic permutation has order 1 or 7. Since the action of f has order 2 on the vertices, it must therefore be an order reversal. It follows that f fixes exactly one vertex of K_7. □

Proposition 4. *For $n \geq 1$, the complete graph K_{4n+3} is intrinsically chiral.*

Proof. Assume that an orientation-reversing homeomorphism $f : \mathbb{R}^3 \to \mathbb{R}^3$ respects some embedding of K_{4n+3}. Let $n_1, \dots, n_p$ denote the lengths of the orbits of the vertices of K_{4n+3} under the action of f. Decompose each n_i as $n_i = 2^{p_i} q_i$ where q_i is odd, and let q be the least common multiple of all the q_i. Set $g = f^q$. Then $g : \mathbb{R}^3 \to \mathbb{R}^3$ is still orientation-reversing, respects K_{4n+3}, and the lengths of the orbits of the vertices under g are all powers of 2 (including $2^0 = 1$).

Since the lengths of the orbits total $4n + 3$ and all orbits have length a power of 2, there must be at least either three orbits of length 1 or one orbit of length 1 and one orbit of length 2. In particular, there is a set of 3 vertices of K_{4n+3} that is invariant under g and fixed pointwise by g^2.

Suppose that there is at least one orbit of length 2^m with $m \geq 2$. Then $g^{2^{m-2}}$ has an orbit of length 4. The union of this orbit with the above g-invariant set of 3 vertices now forms a $g^{2^{m-2}}$-invariant set of 7 vertices of K_{4n+3} and spans a subgraph isomorphic to K_7. Then $g^{2^{m-1}} = (g^{2^{m-2}})^2$ respects this embedding of K_7, acts on its vertices with order 2, and fixes three of its vertices. Since this contradicts the lemma, we conclude that the orbit of each vertex of K_{4n+3} under g must have length 1 or 2.

If the action of g has at least three orbits $\{v_1, v_4\}$, $\{v_2, v_5\}$, $\{v_3, v_6\}$ of length 2, consider the subgraph G of K_{4n+3} consisting of these 6 vertices together with the edges v_1v_2, v_2v_3, v_3v_4, v_4v_5, v_5v_6, v_6v_1 that form a loop and the edges v_1v_4, v_2v_5, v_3v_6 that are the diameters of this loop. Then G is invariant under g. As an abstract graph, however, G is isomorphic to M_3, the Möbius ladder with 3 rungs, and the loop $v_1v_2v_3v_4v_5v_6$ is also invariant under g. In [F] it was proved that for any embedding of M_3 there is no such orientation reversing homeomorphism of S^3 leaving both M_3 and this loop invariant.

If g has only 1 or 2 orbits of length 2, the subgraph of K_{4n+3} spanned by the union of these orbits and of 5 or 3 additional vertices (necessarily fixed by g) provides an embedding of K_7, which contradicts the lemma.

Lastly, if g has no orbit of length 2, it fixes all vertices and edges of K_{4n+3} pointwise. Then g fixes an embedding of the Möbius ladder M_3 as a subgraph of K_{4n+3}, which again contradicts [F], since g is orientation reversing. Hence K_{4n+3} is intrinsically chiral. □

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